DETERMINATION OF g(r), c(r) AND SOME OTHER QUANTITIES IN LIQUID LEAD FROM NEUTRON DIFFRACTION MEASUREMENTS

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The aim of this short paper is the scan of the static phenomena in liquid lead. Therefore, the measurements of $S(\varkappa)$ with the high accuracy on four different temperatures 613, 643, 863 and 1163°K were performed by using the neutron diffractometer at the reactor R2 in Studsvik, Sweden. In order to obtain $S(\varkappa)$ a number of corrections have to be applied to the raw data as background substraction, self-screening, multiple scattering correction, normalization and extrapolation of data smoothly to the value of $S(\varkappa=0)$ over the isothermal compressibility. The corresponding figures of $S(\varkappa)$ with the tabulated $S(\varkappa)$ are given in the report /1/ with many other details. The present data are sufficiently reliable to allow the quantitative comparison with the results of other authors.

The pair correlation function Fig.1), which plays an important role in understanding liquid metals, can be obtained from $S(\varkappa)$ by Fourier transform,

$$g(r)=1+\frac{1}{2\pi^2 rn}\int_0^\infty \left[S(\varkappa)-1\right]\varkappa\sin\varkappa r\,d\varkappa \qquad (1)$$

where n is the average density of atoms.

As was stated previously in some papers, the additional features appear in the pair correlation functions /2/. The subpeaks are supposed to reflect an alternative configuration for the local ordering, which slightly disappears with increasing the temperature. The neutron data of North et al. /3/ showed the same properties in g(r).

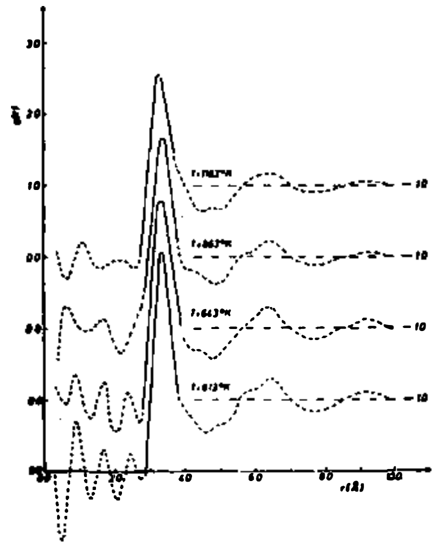

Fig.1

The distribution of atoms as a function of the distance r for a given reference atom at r=0 can be obtained from $S(\varkappa)$ data over the $4\pi r^2 ng(r)$ function. The coordination numbers N_1, N_2 are associated with the area under the peaks of the radial distribution curves $N = 2\int_0^{r_{max}} 4\pi r^2 ng(r)$ where r_{max} is the value of r at the peak.

The direct correlation function c(r) is related to $S(\varkappa)$ by the equation

$$c(r) = \frac{1}{2\pi^2 rn} \int_0^{\infty} \left[\frac{S(\varkappa) - 1}{S(\varkappa)}\right] \varkappa \sin \varkappa r \, d\varkappa \qquad (2)$$

In order to obtain c(r) comparable with Percus-Yevick theory /4/ for the pair potential it is shown that the $\varkappa$-region, to 1.5 $Å^{-1}$, has the greatest importance in the measurements of $S(\varkappa)$.

In many cases the pair potential in liquid metals are similar to the potential of hard-sphere fluid. The structure factor can be calculated for a fluid of hard-spheres according to Percus-Yevick equ. /4/ by the identity

$$S(\varkappa) = \frac{1}{[1 - nc(\varkappa)]} \qquad (3)$$

where $c(\varkappa) = -4\pi \int_0^{\sigma} r^2 dr \frac{\sin \varkappa r}{\varkappa r} \left[\alpha + \beta\left(\frac{r}{\sigma}\right) + \gamma\left(\frac{r}{\sigma}\right)^3\right]$

parameters α , β and γ are a function of the packing fraction /1/. According to the least square fitting procedure the values of hard-sphere diameter were calculated. The fitness is based on the accurate position of the first peak height in the structure factor, as is shown in Fig.2.

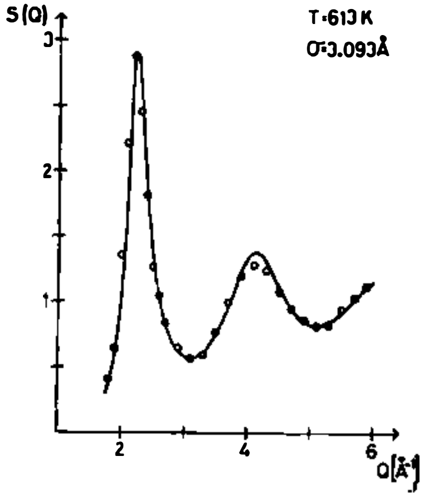

Fig.2

It is obvious that the agreement between the calculated and measured S(κ) are of the order 0.4%. It is stated that the structure factor of S(κ) indicates the hard-sphere behaviour /8/ in liquid metals.

References

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